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Argonne scientists use lasers to align molecules; technique could revolutionize human protein imaging

ARGONNE, Ill. (May 13, 2008) – Protein crystallographers have only scratched the surface of the human proteins important for drug interactions because of difficulties crystallizing the molecules for synchrotron X-ray diffraction. Now scientists at the U.S. Department of Energy's (DOE) Argonne National Laboratory have devised a way to eliminate the need for crystallization by using lasers to align large groups of molecules.

"Strong laser fields can be used to control the behavior of atoms and molecules," Argonne Distinguished Fellow Linda Young said. "Using X-rays, we can investigate their properties in a totally new way."

Crystallization allows scientists to create a periodic structure that will strongly diffract in specific directions when bombarded with X-rays. From the resulting diffraction pattern, scientists can construct a real-space image of the crystal. However, without crystallization, when X-rays collide with multiple, randomly oriented molecules, they diffract in different directions, making it impossible to create a composite diffraction image, said Argonne Physicist Robin Santra.

Some molecules, such as many involved with drug interaction, cannot be crystallized, and imaging would require numerous samples to bombard in order to get a full composite picture. Young's laser technique allows for millions of molecules suspended in a gaseous state to be aligned so that, when bombarded with X-rays, they all diffract in the same way. The resulting images are at atomic level resolution and do not require crystallization.

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Laser-aligned molecules – add one

"Understanding the structure of the approximately 1 million human proteins that cannot be crystallized is perhaps the most important challenge facing structural biology," Young said. "A method for structure determination at atomic resolution without the need to crystallize would be revolutionary."

Young and her team have successfully aligned molecules using a laser, probed the aligned ensemble with X-rays and shown theoretically that the technique could be used for X-ray imaging – see E. R. Peterson et al., *Applied Physics Letters* 92, 094106 (2008) – but they require a proposed upgrade to the Advanced Photon Source facility located at Argonne before X-ray diffraction can be done experimentally.

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